Graphene based electronics and electron 'optics': quantum transport and device opportunities

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Electronic conduction in graphitic materials can be quantitatively understood quite readily using the Landauer transmission theory. We will start by showing that a wide variety of experiments can be explained (Fig. 1) simply in terms of an integral over the mode spectra determined by the density of states, along with an energy-dependent scattering length dictated by Fermi's Golden Rule [1]. The theory, however, needs to be supplemented with a more involved atomistic model when the sheets are narrowed down to nano-ribbon sizes [2]. Using non-orthogonal Extended Huckel Theory, we demonstrate that the edges of narrow armchair nanoribbons resemble benzene minus their resonant stabilization chemistry, imposing thus a molecular property to graphene electronics. The resulting strain along the edges removes any signatures of metallicity, while edge roughness filters out the chiral segments with smaller bandgaps, making the channel width the single arbiter of metallicity. We can thus design wide-narrow-wide all graphene devices monolithically patterned out of a single graphene template [3]. A full solution of Poisson's equation coupled with quantum transport using a fully atomistic non-equilibrium Green's function (NEGF) formalism shows that such a structure benefits from the dual advantages of a superior 2D contact electrostatics as well as a quasi-Ohmic carbon based contact resistance, mitigating short-channel effects that plague modern day silicon devices. However, the bane of these devices, predictably, is their narrow bandgaps that lead to band-to-band tunnelling, once again, consistent with multiple experiments. Our atomistic models allow us to quantify these effects [4].

The electronic gateability of graphene is fundamentally compromised by a trade-off imposed by an asymptotic property of its bandstructure [5]. Atomistic simulations show that on opening a bandgap by various techniques (specifically, selective doping of sheets, quantization in nanoribbons, and the use of transverse fields in Bernally stacked bilayer sheets), the bandstructure stays pinned to a linear dispersion at high energies, so that the bandgap opens not by a simple translation, but by an actual distortion of the bands. Such a distortion fundamentally increases the effective mass all throughout the band, quantifiable in simple terms, leading to a reduction of their mobility even in the absence of any increase in scattering rate. We predict a ~1/Eg reduction the mobility coming from the increase in effective mass alone, and a further ~1/Eg reduction from an increase in scattering length (for bilayer sheets, there is, in addition, a sweet spot due to Van Hove singularities, but the overall trend is still a fundamental reduction in mobility with increasing band-gap). This means that with increase in switching reliability (ie, ON-OFF ratio), there is an invariable reduction in switching speed (ON current), which limits the design space for graphene based electronic switches. Extended to graphene based inverters, we expect accordingly a reduction in gain, a reduced voltage swing and a poor saturation of the transfer characteristics, in close quantitative agreement with experiments [6].

A question we raise at the end is whether it is at all possible to design a graphene based switch without structurally distorting it in the process of opening a band-gap. We show that this is in principle possible using purely geometrical means, exploiting the pseudospin structure of the phase-coupled graphitic conduction and valence bands. It is, in fact, this property that fundamentally distinguishes graphene from other 2D semiconductors such as silicon inversion layers, boron nitride or molybdenum disulfide. In all narrow-bandgap semiconductors, a low voltage band-to-band tunneling causes electrons to follow trajectories reminiscent of Snell's law in optics, albeit with a 'refractive index' that can be gate tuned into negativity. However, it is the pseudospin structure that determines the strength and angular quenching of the refracted and reflected waves (the equivalent of Fresnel coefficients in optics) – in other words, Klein-antiKlein tunneling in regular or bilayer sheets. In fact, we can see how this pseudospin rotates as we incrementally open a bandgap and thereby introduce a pseudo-magnetic field. Our results compare well with recent experiments that show how this pseudospin selectivity controls a graphene pn junction resistance (both on exfoliated and CVD grown samples), with varying tilt angles.

The theoretical and experimental gateability of a Klein tunnel switch is still quite modest to be of interest from a device switching perspective. What we argue is that by introducing an additional scattering barrier from a non-graphitic structure (e.g. a cut in a graphene sheet), we can introduce a transmission gap that arises when the angle subtended by the cut at the source exceeds the critical angle for the graphene electrons. Aside from introducing a large ON-OFF ratio, the significant development is that this gap can be collapsed by reducing the voltage gradient across the junction [7]. Such a gate tunable

metal insulator transition does two things – it eliminates the current on the heterogeneous PN side of the voltage axis [8], and significantly sharpens the rising current on the homogeneous PP or NN side, in fact, exceeding the thermodynamic limit imposed by Boltzmann statistics that limits present day silicon based transistors. The unipolar, sub-thermal switch (Fig. 1) arises simply because we can tune the transmission gap of the heterostructure with a gate voltage, a property once again, unique to graphene and its pseudospin structure. We show how it allows us to design a high quality inverter that can operate at a higher frequency [9]. We also show how the ability to control the electron trajectory helps create reconfigurable electronic devices based on graphene heterojunctions.

The gate tunability of the gap is supported by fully atomistic simulations of current flow through large (~200x600nm) sheets. However, these simulations also emphasize how sensitive graphene based electron 'optics' tends to be, outlining three significant challenges that need to be overcome – (i) we need ways to collimate the electrons without significantly excising their modal density and reducing the ON currents; (ii) we need ways to create high quality sheets and patterned contacts to avoid unintentional rotations of the pseudospins from pseudo-magnetic fields at these junctions; and (iii) most significantly, we need ways to flush out the electrons at the edges, which otherwise tend to redirect the electrons back towards the junctions and create large, dissipative leakage paths.

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Figures

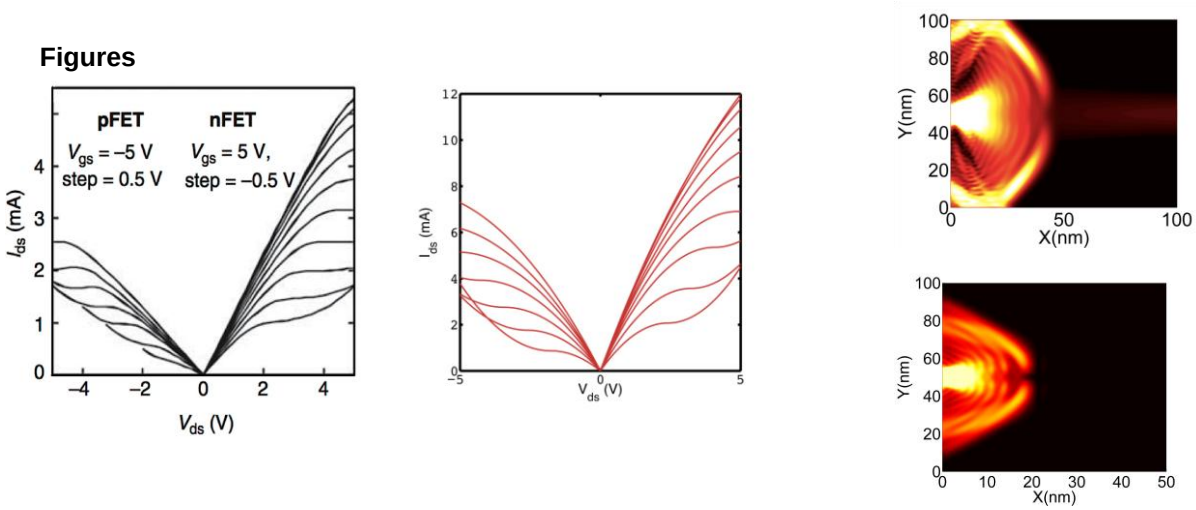

Fig. 1. (Left) Experiments and (center) theory [1] showing graphene I-Vs with contact induced asymmetry and band-to-band tunneling. (Right) atomistic simulations show that across a graphene heterojunction with a split gate, electronic transmission can be quenched by the geometrical property of the pseudospin states (top) and completely eliminated with a regular (as opposed to Klein) tunnel barrier in the graphene structure, using a cut for instance [9].